WHAT IS CLAIMED IS:

1. A composition comprising a *E. coli* FabH in crystalline form.

2. The composition according to claim 1 wherein said FabH is a dimer.

3. The composition according to claim 1 wherein said FabH comprises an active site cavity formed by amino acids comprising Cys112, His244 and Asn274

4. The composition of claim 1 wherein said FabH is a *E. coli* FabH.

5. The composition of claim 3 wherein said FabH is characterized by the coordinates selected from the group consisting of the coordinates of Figures 1-2 and Tables I, II, and III.

6. A *E. coli* FabH crystal.

7. A selenomethionine mutant crystal of a *E. coli* FabH.

8. An isolated, properly folded FabH molecule or fragment thereof having a conformation comprising the protein coordinates of Figures 1-2 and Tables I, II, and III.

9. The molecule according to claim 8 wherein said molecule is a dimer, wherein each monomer is characterized by two similar domains having core of five β-strands, each containing flanking helices, strands and loops, as illustrated in Fig. 3.

10. The molecule according to claim 8 wherein said molecule is a dimer characterized by the dimer interface of Fig. 3.

11. The molecule according to claim 10 which is *E. coli* FabH.

12. A peptide, peptidomimetic or synthetic molecule which interacts competitively or non-competitively with the active site of a FabH of claim 1.

13. A method of identifying an inhibitor compound capable of binding to, and inhibiting the enzymatic activity of, a *E. coli* FabH, said method comprising: introducing into a suitable computer program information defining an active site conformation of a *E. coli* FabH molecule comprising a conformation defined by the coordinates of Figures 1-2 and Tables I, II, and III, wherein said program displays the three-dimensional structure thereof; creating a three dimensional structure of a test compound in said computer program; displaying and superimposing the model of said test compound on the model of said active site; assessing whether said test compound model fits spatially into the active site; incorporating said test compound in a biological activity assay for a FabH characterized by said active site; and determining whether said test compound inhibits enzymatic activity in said assay.

14. The method according to claim 13 wherein said FabH molecule is a dimer, wherein each monomer is characterized by two similar domains having core of five β-strands, each containing flanking helices, strands and loops, as illustrated in Fig. 3.

15. A method of identifying an inhibitor compound capable of binding to, and inhibiting the enzymatic activity of, a *E. coli* FabH, said method comprising: introducing into a suitable computer program information defining an active site conformation of a FabH molecule comprising a conformation defined by the coordinates of Figures 1-2 and Tables I, II, and III, wherein said program displays the three-dimensional structure thereof; creating a three dimensional structure of a test compound in said computer program; displaying and superimposing the model of said test compound on the model of said active site; assessing whether said test compound model fits spatially into the active site; incorporating said test compound in a biological activity assay for a FabH characterized by said active site; and determining whether said test compound inhibits enzymatic activity in said assay.

16. The method according to claim 15 wherein said FabH molecule is a dimer, wherein each monomer is characterized by two similar domains having core of five β-strands, each containing flanking helices, strands and loops, as illustrated in Fig. 3.

17. A peptide, peptidomimetic or synthetic molecule identified by the method of claim 13 or 15.

18. A method for solving a crystal form comprising using the structural coordinates of a *E. coli* FabH crystal or portions thereof, to solve a crystal form of a mutant, homologue or co-complex of said FabH by molecular rearrangement.

19. A method of drug design comprising the step of using the structural coordinates of a *E. coli* FabH crystal to computationally evaluate a chemical entity for associating with the active site and substrate binding sites of *E. coli* FabH.

20. The method of drug design according to claim 19 comprising the step of using the structure coordinates of *E. coli* FabH to identify an intermediate in a chemical reaction between said FabH and a compound with is a substrate or inhibitor of said enzyme.

21. The method according to claim 20, wherein said entity is a competitive or non-competitive inhibitor of a *E. coli* FabH.

22. The method of drug design according to claim 19, using the structure of a FabH homologue that has similar amino acid identities as well as spacial arrangements as those of *E. coli* FabH listed in Tables I-III.

23. The method of drug design according to claim 20 using the structure of a FabH homologue that has similar amino acid identities as well as spacial arrangements as those of *E. coli* FabH listed in Tables I-III.

24. The method of drug design according to claim 21 using the structure of a FabH homologue that has similar amino acid identities as well as spacial arrangements as those of *E. coli* FabH listed in Tables I-III.

25. The method according to claim 19 wherein said structure coordinates comprise the coordinates of Figures 1-2 and Tables I, II, and III.

26. The method according to claim 20 wherein said structure coordinates comprise the coordinates of Figures 1-2 and Tables I, II, and III.

27. The method according to claim 21 wherein said structure coordinates comprise the coordinates of Figures 1-2 and Tables I, II, and III.